Combinatorics, wreath products, finite space groups and magnetism

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In this lecture some mathematical tools necessary for a proper description of the Heisenberg antiferromagnet are presented. We would like to point out differences between ferro- and antiferromagnetic cases of Heisenberg Hamiltonian for finite spin systems. The ground–state properties are discussed.

I. INTRODUCTION

The Heisenberg model of magnetism has been investigated for years. For the finite spin system consisting of $N < \infty$ spins $\vec{s}$ we obtain the following formula

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{s}_i \vec{s}_j - h \sum_i s_i^z \tag{1}$$

where the first sum is taken over all nearest-neighbor pairs $\langle ij \rangle$ and h is an external magnetic field parallel to z-axis (number of the nearest-neighbor pairs will be denoted hereafter as $\mathcal{N}$).

A. Ferromagnet ($J > 0$)

The ground state of the finite Heisenberg ferromagnet has the following properties:

- for $h = 0$ the ground state is $(2Ns + 1)$-tuplet with total spin number $S = Ns$ and energy per spin $\mathcal{E}_0^+ = -J\mathcal{N}s^2/N$;
- For $h > 0$ the above multiplet splits into singlets and the ground-state is the one of them with maximal magnetization $M = Ns$ and the energy per site $\mathcal{E}_h^+ = \mathcal{E}_0^+ - hs$;
- the energy gap $\Delta\mathcal{E}^+$ between the ground state and the first excited state is equal to h/N, so it is proportional to h.

The above properties agree with the classical results (all spins are 'parallel') and with the thermodynamic limit $(N \longrightarrow \infty,\ h \longrightarrow 0)$.

B. Antiferromagnet ($J < 0$)

The classical ground state of antiferromagnet is described by the so-called Néel state configuration $|s\ -s\, s \ldots s\ -s\rangle$. It is evident that this state has two-fold degeneracy. If one defines (see[1]) the Néel state as a state with opposite magnetizations in (ferromagnetic) sublattices (i.e. $S_A = S_B = Ns/2$ and $M_A = -M_B$), then the degeneracy of this state is $Ns + 1$. On the other hand Marshall and Peirels have proved that the ground state of antiferromagnet is a singlet with $S = M = 0$[2]. Moreover, simple calculations for finite spin systems show that the ground state has the following properties

- the ground state is a singlet even for $h = 0$;
- the ground state is a linear combination of all states with total magnetization $M = 0$;
- the energy gap $\Delta\mathcal{E}^-$ decreases for increasing $h > 0$ and for sufficient large h the ground state is a state with $S = M = 1$ (for very large h in the ground state $S = M = Ns$ — the ferromagnetic ground state is obtained).

C. Finite Lattice Method

Considerations of finite spin systems is very popular and effective method, therefore it has been frequently applied since the pioneer work of Bonner and Fisher[3]. Number of states, which should be considered, is $(2s+1)^N$, so it grows very quickly (for $s = 1/2$ and 4×4 square lattice there are $2^{16} = 65536$ states!). Therefore a lot of methods are used in order to decrease a dimension of the Hamiltonian eigenproblem or to simplify the solving procedure (e.g. Lanczos method[4], combinatorial methods[1] and group-theoretical method[5]). In the last case a translation group of considered lattice is taken into account, as a rule. In contrary, we investigate also a point group and a space group (of finite lattice), therefore a more complete state classification scheme can be obtained[6].

1. Example: Four spins $s = 1/2$ with the periodic boundary conditions

In this case the translation group is $\mathcal{T} = C_4$, the point group is $\mathcal{P} = \{E, \sigma\} = C_s$ and the space group — $\mathcal{S} = C_{4v}$. Classification scheme for $2^4 = 16$ states is given in Tab.I. $\mathcal{E}$ denotes the energy per spin, S, M — total spin number and magnetization, respectively, and $\Theta \in \{\Theta_{-1}, \Theta_0, \Theta_1, \Theta_2\}$, $\Xi \in \{\Xi_0, \Xi_1\}$ and $\Gamma \in \{A_1, A_2, B_1, B_2, E\}$ are the irreps of C_4, C_s and C_{4v}, respectively. It is worth noting that two possible decompositions of the irrep $E = \Theta_{-1} \oplus \Theta_1 = \Xi_0 \oplus \Xi_1$ correspond to two choices of the basis in the irreducible subspace labelled by E. In the first case the basis is complex and in the second — real one, respectively. In other words all states labelled by E correspond to wave vector with $|\vec{k}| = 1$ but in the first case there is additional index — $\mathrm{sign} k = \pm 1$, and in the second — a symmetry index $\alpha = \pm 1$ (i.e. $\sigma\,|E\alpha\rangle = \alpha\,|E\alpha\rangle$, where $\sigma \in \mathcal{P}$ is a reflection). The (antiferromagnetic) ground state is given as a linear combination

$$\frac{\sqrt{3}}{3}\left(|+-+-\rangle + |-+-+\rangle\right) - \frac{\sqrt{3}}{6}\left(|++--\rangle + |+--+\rangle + |--++\rangle + |-++-\rangle\right). \tag{2}$$

TABLE I. Classification of states for 4 spins 1/2, $J = -1$

Θ	Γ	Ξ	S	M	$\mathcal{E}$	Degeneracy	
						$h = 0$	$h \neq 0$
Θ_0	A_1	Ξ_0	0	0	-0.50	1	1
Θ_2	B_1	Ξ_0	1	0	-0.25	1	1
Θ_2	B_1	Ξ_0	1	±1	$-0.25(1 \pm h)$	2	1+1
Θ_2	B_2	Ξ_1	0	0	0.00	1	1
$\Theta_{-1} \oplus \Theta_1$	E	$\Xi_0 \oplus \Xi_1$	1	0	0.00	2	2
$\Theta_{-1} \oplus \Theta_1$	E	$\Xi_0 \oplus \Xi_1$	1	±1	$\mp 0.25h$	4	2+2
Θ_0	A_1	Ξ_0	2	0	0.25	1	1
Θ_0	A_1	Ξ_0	2	±1	$0.25(1 \mp h)$	2	1+1
Θ_0	A_1	Ξ_0	2	±2	$0.25(1 \mp 2h)$	2	1+1

II. METHOD

A. Short Description

The most important aim of our work is to determine the ground state of (finite) Heisenberg antiferromagnet and its properties. It has been done for spin systems with $s = 1/2$ and a linear chain up to 16 spins, square 4×4 lattice, and a $2 \times 2 \times 2$ cube. The results and the detail description is presented elsewhere (see[7]). The main points of used procedure are following

1. Find number N_0 of states with total magnetization $M = 0$ (more precisely — we calculate a dimension of subspace L_0 containing such states);
2. Determine this states, i.e. determine the basis $\mathcal{B}$ in the subspace L_0;
3. Decompose this basis into orbits of the space group (since the space group $\mathcal{S}$ is a subgroup of the symmetry group Σ_N, then one can consider the action of Σ_N on $\mathcal{B}$);
4. It can be proved that when Ns is even number then the ground state is "fully" symmetric (i.e. it transforms as the unit irrep), therefore from each subspace spanned on a given orbit one (the unique) such state is chosen;
5. The eigenproblem for the operator $\vec{S}^2$ (square of total spin $\vec{S}$) is solved for these states (the eigenvalues of this operator are $0, 2, 6, \ldots, Ns(Ns+1)$ and the equation $\vec{S}^2 \left|\psi\right\rangle = 0$ is the most interesting);
6. After the above presented steps the states labelled by $M = 0$, $\Gamma = \Gamma_0$, and $S = 0$ are obtained and the ground state is a linear combination of these states — it is determined by solution of the eigenproblem $\mathcal{H} \left|\varphi\right\rangle = \mathcal{E} \left|\varphi\right\rangle$;
7. As a result the ground state is obtained as a linear combination of the so-called Ising configurations and its properties can be easily determined (e.g. spin-spin correlations, staggered magnetization, etc.).

It should be underlined that this procedure gives only the ground state, therefore the thermodynamics properties of the considered system cannot be determined. These properties can be found when one solves eigenproblems for each total spin number $S = 0, 1, 2, \ldots, Ns$ and for each irrep of the space group.

B. Combinatorics

The first three steps can be done applying combinatorial methods. The problem is: 'Find all states with a given magnetization, i.e. states $\left|m_1 m_2 \ldots m_N\right\rangle$ fulfilling the condition $\sum_i m_i = M$'. Since the magnetization operator $S^z = \sum_i s_i^z$ commutes with any $\sigma \in \Sigma_N$, then the action of Σ_N on the set $\{1, 2, \ldots, N\}$ can be considered. In the simplest case $s = 1/2$ number of states with the magnetization equal M is given by the binomial coefficient

$$\dim L_M = \binom{N}{\frac{N}{2} + M}$$

where $k = N/2 + M$ is a number of spins with a projection $m = 1/2$. For $s > 1/2$ it can be generalized by the polynomial coefficient[8]

$$\binom{N}{n_0 n_1 \ldots n_{2s}} = \frac{N!}{n_0! n_1! \ldots n_{2s}!}; \quad \sum_{i=0}^{2s} n_i = N$$

where n_i denotes number of spins with projection $i - s$. Number of states is determined by the following sum

$$\dim L_M = \sum_{(n_0 n_1 \ldots n_{2s})} \binom{N}{n_0 n_1 \ldots n_{2s}}$$

taking over all decompositions $(n_0 n_1 \ldots n_{2s})$ with the condition $\sum_i n_i (i - s) = M$. For example, for $N = 3$, $s = 1$, and $M = 0$ one obtains

$$\dim L_0 = \binom{3}{111} + \binom{3}{030} = 7.$$

C. Finite space groups

The fourth step of our procedure is to determine symmetry adapted basis of subspace L_0 according to the symmetry group of the considered Hamiltonian. It means, that only these permutations $\sigma \in \Sigma_N$ are taking into account which preserve order of points ('neighborhood). These elements form (finite) space group of finite lattice. It can be shown that in the one-dimensional case it is the group $C_{Nv} = C_N \Box C_s = D_N$. From it follows that for a hypercubic lattice in d-dimensional space the space group is given as a wreath product[9]

$$\mathcal{S} = C_{Nv} \wr \Sigma_d$$

where elements of the symmetric group Σ_d permute axes of d-dimensional coordinate system. The above group is called a *complete monomial group (of degree d) of the group C_{Nv}*. The considerations of a linear representations of this group in the subspace L_0 give us the appropriate symmetry adapted basis, which is used in the next steps of our procedure (5–7). These steps are performed using numerical methods (solution of eigenproblem for real symmetric matrix).

III. FINAL REMARKS

Using the above described method we have obtained, e.g., energy per site for 16-spin linear chain. Its value — -0.446 — is very close to the exact result in the thermodynamic limit — $1/4 - \ln 2 \approx -0.4432$. Therefore, one can say that in the one-dimensional case a system of 20 spins is quite good approximation of the infinite system.

Application of the proposed procedure to two- and three-dimensional spin systems requires much more intensive investigations of group action of the symmetric group Σ_N on the basis states (the Ising configurations) $|m_1 \dots m_N\rangle$. It should enable to consider system of 20×20 or $10 \times 10 \times 10$ spins for any value of spin number s.

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[1] P.L. Iske and W.J. Caspers, *Physica* **142A** (1987) 360.
[2] W. Marshall, *Proc. Roy. Soc. (London)* **A232** (1955) 48.
[3] J.C. Bonner and M.E. Fisher, *Phys. Rev.* **135** (1964) A641.
[4] A. Moreo, *Phys. Rev.* **B35** (1987) 8562.
[5] P.M. Duxburry and J. Oitmaa, *J. Phys. C: Solid State Phys.* **16** (1983) 4199.
[6] T. Lulek, *J. de Physique* **45** (1984) 29; W. Florek and T. Lulek, *J. Phys. A: Math. Gen.* **20** (1987) 1921.
[7] W. Florek, *Acta Magnetica: Supplement* (1990) 114; W. Florek, *Acta Mag.* **VIII** (1991) 25.
[8] W. Florek, *Acta Mag.* **II** (1985) 43, ibid. **V** (1988) 145.
[9] W. Florek, in: W. Florek, T. Lulek, and M. Mucha (eds.), *Proceedings of the International School on Symmetry and Structural Properties of Condensed Matter*, World Scientific, Singapore, 1991, p. 365.